(FILE 'HOME' ENTERED AT 08:24:10 ON 14 OCT 2004) FILE 'CASREACT' ENTERED AT 08:26:21 ON 14 OCT 2004 STRUCTURE UPLOADED L10 S L1 L2 1 S L1 FUL L3 STRUCTURE UPLOADED L40 S L4 L51 S L4 FUL L6 FILE 'CAPLUS' ENTERED AT 08:35:44 ON 14 OCT 2004 389101 S COUPLING L71570 S ARYL BROMIDE# 18 L94345 S ARYL HALIDE# 5458 S L8 OR L9 L10198737 S KETONE# L11389101 S L7 L12140 S L7 AND L10 AND L11 L13143277 S PALLADIUM L1482 S L14 AND L13 L155173 S BRONSTED L16 614351 S BRONSTED OR BASE L17 15 S L17 AND L15 L18=> d bib abs kwic 1-15ANSWER 1 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN L18 2004:218750 CAPLUS ANDN140:253348 Preparation of biaryls from aryl halides and arylboranes Nishida, Mayumi; Tagata, Takeshi INKoei Chemical Co., Ltd., Japan PA Jpn. Kokai Tokkyo Koho, 16 pp. SO CODEN: JKXXAF DTPatent Japanese LA FAN.CNT 1 APPLICATION NO. DATE KIND DATE PATENT NO. ____ JP 2002-249649 20020828 A2 20040318 JP 2004083530 $_{
m PI}$ 20020828 PRAI JP 2002-249649 OS MARPAT 140:253348 Biaryls are prepared by reaction of aryl halides with AΒ arylboronic acids or dialkylarylboranes in solvents in the presence of (a) Pd catalysts, which are insol. in solvents and show specific x-ray photoelectron spectra, (b) bases, and (c) phosphines. P-ClC6H4CN was treated with PhB(OH)2 in 1,2-dimethoxyethane in the presence of PPh3, KHCO3, and Pd/C at 80° for 8 h to give 67% 4-cyanobiphenyl. Preparation of biaryls from aryl halides and TIarylboranes Biaryls are prepared by reaction of aryl halides with AΒ arylboronic acids or dialkylarylboranes in solvents in the presence of (a) Pd catalysts, which are insol. in solvents and show specific x-ray photoelectron spectra, (b) bases, and (c) phosphines. P-ClC6H4CN was treated with PhB(OH)2 in 1,2-dimethoxyethane in the presence of PPh3, KHCO3, and Pd/C at 80° for 8 h to give 67% 4-cyanobiphenyl. biaryl prepn aryl halide coupling STarylborane; palladium catalyst aryl halide coupling arylborane; phosphine base palladium

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FILE 'CASREACT' ENTERED AT 08:26:21 ON 14 OCT 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 1 S L1 FUL

=> d bib abs crd 13

L3 ANSWER 1 OF 1 CASREACT COPYRIGHT 2004 ACS on STN

AN 108:94141 CASREACT

TI 2-Ethynylbenzenealkanamines. A new class of calcium entry blockers

AU Carson, J. R.; Almond, H. R.; Brannan, M. D.; Carmosin, R. J.; Flaim, S. F.; Gill, A.; Gleason, M. M.; Keely, S. L.; Ludovici, D. W.; et al.

CS McNeil Pharm., Spring House, PA, 19477-0776, USA

Journal of Medicinal Chemistry (1988), 31(3), 630-6

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

GΙ

MeO
$$C\equiv CPh$$
 OMe $(CH_2)_2CHMeNMe(CH_2)_2$ OMe

AB A series of 2-[aryl(alkyl)ethynyl]benzenealkanamines was synthesized. The compds. exhibit antihypertensive activity in spontaneously hypertensive rats and coronary vasodilator activity with minimal neg. inotropic activity in the Langendorff guinea pig heart in vitro. They exert their activity by inhibition of Ca2+ influx across cell membranes. Optimal activity is found among the N-(arylethyl)-5-methoxy-α-methyl-2- (phenylethynyl)benzeneethanamines and -propanamines, e.g., I.

Ι

RX(25) OF 149

=> d his

(FILE 'HOME' ENTERED AT 08:24:10 ON 14 OCT 2004)

FILE 'CASREACT' ENTERED AT 08:26:21 ON 14 OCT 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 1 S L1 FUL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 1 S L4 FUL

=> d crd bib

L6 ANSWER 1 OF 1 CASREACT COPYRIGHT 2004 ACS on STN

RX(3) OF 149

RX(25) OF 149

AN 108:94141 CASREACT

TI 2-Ethynylbenzenealkanamines. A new class of calcium entry blockers

AU Carson, J. R.; Almond, H. R.; Brannan, M. D.; Carmosin, R. J.; Flaim, S. F.; Gill, A.; Gleason, M. M.; Keely, S. L.; Ludovici, D. W.; et al.

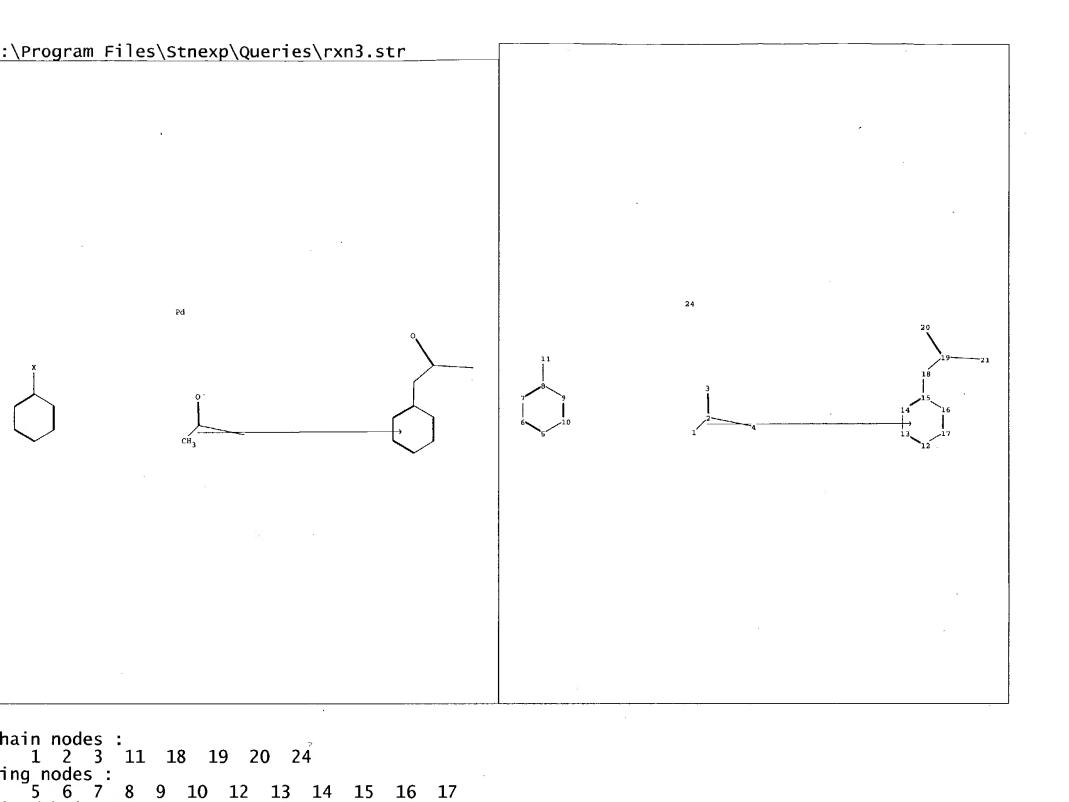
CS McNeil Pharm., Spring House, PA, 19477-0776, USA

SO Journal of Medicinal Chemistry (1988), 31(3), 630-6 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

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1-2 2-3 2-4 8-11 15-18 18-19 19-20 19-21
ing bonds :
  5-6 5-10 6-7 7-8 8-9 9-10 12-13 12-17 13-14 14-15 15-16 16-17
xact/norm bonds :
 2-3 19-20
xact bonds :
  1-2 2-4 8-11 15-18 18-19 19-21
ormalized bonds :
  5-6 5-10 6-7 7-8 8-9 9-10 12-13 12-17 13-14 14-15 15-16 16-17
atch level :
  1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
  11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
  20:CLASS 21:CLASS 24:CLASS
ragments assigned reagent role:
  containing 24
ragments assigned product role:
  containing 12
ragments assigned reactant/reagent role:
  containing 1 containing 5
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ing/chain nodes :

4 21 hain bonds :